Surface Modification Solutions for a plethora of applications

Glass  Energy  Textiles  Displays  Ceramics  Digital Inks  Thermosets  Biomaterials  Printing Inks  Quantum Dots  Semiconductor  Thermoplastic  Chromatography  Nano-Composites  Imaging & Printing  Advanced Composites  Optics & Optoelectronics

Understanding characteristics that may affect the performance of surface modified micro-particles can dramatically improve the performance in many applications and markets:

**Micro-Particle Surface Modification**

**Micro-Particle Properties**
- morphology
- crystal lattice
- polymorphism
- semiconductive
- surface characteristics

**Micro-Particle Dramatic Effects**
- rheological behavior
- hiding power, color strength
- dispersion, solubility, polarity
- photo, chemical, thermal stability
- mechanical & electrical properties
- moisture & corrosion resistance

**Gelest, Inc.**
provides focused technical solutions for surface modification applications and maintains the capabilities to handle flammable, corrosive and air sensitive materials. Headquartered in Morrisville, PA Gelest is recognized worldwide as an innovator, manufacturer and supplier of commercial and research quantities of silanes, metal-organics and silicones, serving advanced technology markets through a material science driven approach.

For additional information on Gelest’s Surface Modification Technology or to inquire on how we may assist in *Enabling Your Technology*, please contact:

**Gelest**
www.gelest.com
11 East Steel Rd.
Morrisville, PA 19067
Phone: 215-547-1015
Fax: 215-547-2494
micro-particle@gelest.com

© 2009 Gelest, Inc.
Innovating Particle Functionalization

Gelest, Inc. provides focused technical solutions for surface modification applications and maintains the capabilities to handle flammable, corrosive and air sensitive materials. Headquartered in Morrisville, PA Gelest is recognized worldwide as an innovator, manufacturer and supplier of commercial and research quantities of silanes, metal-organics and silicones, serving advanced technology markets through a material science driven approach.

Gelest Provides Chemistries and Deposition Technologies that Dramatically Enhance:
- Color
- Polarity
- Adhesion
- Dispersion
- Rheological Behavior
- Photo, Chemical, Thermal Stability
- Moisture & Corrosion Resistance
- Mechanical & Electrical Properties
**Surface Modification Solutions**

**COUPLING THE PARTICLE TO THE APPLICATION**

**Chemical Considerations**

**INPUTS**
- Particle
  - Natural
  - Synthetic
  - Siliceous
  - Non-siliceous

**PHYSICAL PROPERTIES**
- Particle Size Distribution
- Density
- Aspect Ratio
- Contact Angle

**Surface Properties**
- Oleophilicity
- Oleophobicity
- Zeta Potential
- Hydrophilicity
- Hydrophobicity

**Bonding Mechanisms**
- Ionic Bonding
- Metallic Bonding
- Covalent Bonding
- Aromatic Bonding
- Acid Base Interactions
- Hydrogen Bonding

**Wettability & Surface Area Effects**
- Interpenetrating Polymeric Networks

**Silane Effectiveness on Inorganic Substrates**

<table>
<thead>
<tr>
<th>Substrate</th>
<th>Excellent</th>
<th>Good</th>
<th>Poor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chabazite</td>
<td>Pyrophyllite</td>
<td>Quartz</td>
<td>Kaolinite</td>
</tr>
<tr>
<td>Hectorite</td>
<td>Lepidolite</td>
<td>Smectite</td>
<td>Attapulgite</td>
</tr>
</tbody>
</table>

**Solutions**

Adapted from a Digipal phase diagram of chlorosilanes, methoxysilanes, and cyclic azasilanes in order to perform small particle and nano-sized substrates. Chloroform, methanol, or other organic solvents are often used to promote silane deposition. The temperature is adjusted to 30-150°C, depending on the substrate to be treated.

**Bonding Mechanisms**

1. **Oleophilicity**: Attraction to hydrocarbons.
2. **Oleophobicity**: Repulsion from hydrocarbons.
4. **Hydrophilicity**: Attraction to water.
5. **Hydrophobicity**: Repulsion from water.

**Surface Properties**

- **Oleophilicity**: Attraction to hydrocarbons.
- **Oleophobicity**: Repulsion from hydrocarbons.
- **Zeta Potential**: Measurement of the electrical double layer.
- **Hydrophilicity**: Attraction to water.
- **Hydrophobicity**: Repulsion from water.

**Bonding Mechanisms**

- **Ionic Bonding**: Electrostatic attraction between ions.
- **Metallic Bonding**: Covalent bonding in metal crystals.
- **Covalent Bonding**: Strong chemical bonding.
- **Aromatic Bonding**: Delocalized pi electrons.
- **Hydrogen Bonding**: Hydrogen bonding.
- **Acid Base Interactions**: Charge transfer.

**Chemical Considerations**

- **Solid Surface**: Interaction with the substrate.
- **Chemisorption**: Chemical bonding.
- **Electrostatic**: Charge transfer.
- **Contact Angle**: Water contact angle.
- **Mobility**: Movement of the particle.
- **Density**: Material density.
- **Aspect Ratio**: Shape of the particle.

**Surface Properties**

- **Contact Angle**: Measurement of the hydrophilicity.
- **Mobility**: Movement of the particle.
- **Density**: Material density.
- **Aspect Ratio**: Shape of the particle.

**Bonding Mechanisms**

- **Ionic Bonding**: Electrostatic attraction between ions.
- **Metallic Bonding**: Covalent bonding in metal crystals.
- **Covalent Bonding**: Strong chemical bonding.
- **Aromatic Bonding**: Delocalized pi electrons.
- **Hydrogen Bonding**: Hydrogen bonding.
- **Acid Base Interactions**: Charge transfer.

**Silane Effectiveness on Inorganic Substrates**

**EXCELLENT**
- Glauberite
- Glass
- Aluminum (Al2O3)
- Alumino-silicates (e.g., clays)

**GOOD**
- Zeolite
- Talc
- Phlogopite Mica
- Montmorillonite
- Chabazite

**POOR**
- Diatomite
- Pyrophyllite

**Surface Modification Solutions**

**COUPLING THE PARTICLE TO THE APPLICATION**

**Surface Properties**

- **Oleophilicity**: Attraction to hydrocarbons.
- **Oleophobicity**: Repulsion from hydrocarbons.
- **Zeta Potential**: Measurement of the electrical double layer.
- **Hydrophilicity**: Attraction to water.
- **Hydrophobicity**: Repulsion from water.

**Bonding Mechanisms**

- **Ionic Bonding**: Electrostatic attraction between ions.
- **Metallic Bonding**: Covalent bonding in metal crystals.
- **Covalent Bonding**: Strong chemical bonding.
- **Aromatic Bonding**: Delocalized pi electrons.
- **Hydrogen Bonding**: Hydrogen bonding.
- **Acid Base Interactions**: Charge transfer.

**Chemical Considerations**

- **Solid Surface**: Interaction with the substrate.
- **Chemisorption**: Chemical bonding.
- **Electrostatic**: Charge transfer.
- **Contact Angle**: Water contact angle.
- **Mobility**: Movement of the particle.
- **Density**: Material density.
- **Aspect Ratio**: Shape of the particle.

**Surface Properties**

- **Contact Angle**: Measurement of the hydrophilicity.
- **Mobility**: Movement of the particle.
- **Density**: Material density.
- **Aspect Ratio**: Shape of the particle.

**Bonding Mechanisms**

- **Ionic Bonding**: Electrostatic attraction between ions.
- **Metallic Bonding**: Covalent bonding in metal crystals.
- **Covalent Bonding**: Strong chemical bonding.
- **Aromatic Bonding**: Delocalized pi electrons.
- **Hydrogen Bonding**: Hydrogen bonding.
- **Acid Base Interactions**: Charge transfer.
**Surface Modification Solutions**

**COPPING THE PARTICLE TO THE APPLICATION**

**INPUTS**

- **Couplant**
- **Substrate**

**CHEMICAL CONSIDERATIONS**

- Talc
- Clinoptilolite

**Surface Properties**

- **Oleophilicity**
- **Oleophobicity**
- **Zeta Potential**
- **Hydrophobicity**
- **Hydrophilicity**
- **Contact Angle**

**Bonding Mechanisms**

- **Ionic Bonding**
- **Metallic Bonding**
- **Covalent Bonding**
- **Aromatic Bonding**
- **Hydrogen Bonding**
- **Acid Base Interactions**

**Surface Modification Solutions**

- **Specialty**
  - Non-siliceous
  - Siliceous

**Particle**

- **SILICEOUS**
  - natural
  - synthetic
  - NON-SILICEOUS
  - synthetic

**Physical Properties**

- **Density**
- **Aspect Ratio**
- **Surface Area**
- **Contact Angle**
- **Chemisorption**
- **Electrothermic Mobility**

**Pore Size & Volume**

**Particle Size Distribution**

**Silane Effectiveness**

- **One Monolayer**
  - SUBSTRATES
- **One Polylayer**
  - SUBSTRATES

**Solutions**

- **Polymer**
  - Mixed Deposition
  - Layer-by-Layer Deposition

**Monolayer Polylayer**

**Amine Biomolecules**

- are used for binding or surface modification of inorganic particles.

**Polymer Blends**

- are used in composite formulations. In this method the silane is used as a simple additive. Compounds can be prepared by the introduction of alkoxysilanes to dry-blends of polymer and filler prior to compounding. Generally 0.5 to 2.0 weight percent of silane in the total polymer is dispersed by spraying the silane in an alcohol carrier onto a preblend. The addition of the alkoxysilanes is diluted with the solvent of choice to yield a homogeneous mixture. The mixture is then dried by heating and then melt compounded. This method is most effective if the filler is in powders or the blending of the top layer of treated material is achieved by using air or steam flow.

**Silane Deposition**

- silanes can be applied to substrates under dry aprotic conditions by chemical vapor deposition methods. These methods favor monolayer deposition. Although under proper conditions alkoxysilanes can be deposited to the vapor phase, these usually contain 5% to 20% of the substrate to be treated. It is washed with the solvent. The solvent is then removed by air or explosion of even drying. No further processing is necessary. The reaction involves a direct nucleophilic displacement of the chloride ion by HCl or methoxide as methanol by the surface silanol. If monolayer deposition is desired, substrates should be prepared at 110°C for 4-6 hours. Bulk deposition methods also use water to promote the silane. This method is more effective for large scale preparations and rigorous controls must be established to ensure reproducible results. More reproducible coating is obtained with monomer- chlorosilanes.

- Bulk deposition onto powders, e.g. fillers, is usually accompanied by a spray-on method. In this method the substrate is first treated in an aqueous solution of silane. The mixture is refluxed for 12-24 hours with intensive mixing. After the reaction is finished, the substrate is washed with the solvent. The solvent is then removed by air or explosion of even drying. No further processing is necessary. The reaction involves a direct nucleophilic displacement of the chloride ion by HCl or methoxide as methanol by the surface silanol. If monolayer deposition is desired, substrates should be prepared at 110°C for 4-6 hours. Bulk deposition methods also use water to promote the silane. This method is more effective for large scale preparations and rigorous controls must be established to ensure reproducible results. More reproducible coating is obtained with monomer- chlorosilanes.

**Surface Modification Applications**

- Adhesive and Paper Liquid deposition: adhesives, thermosets, hot melts and cold sets are used for various applications. The bond strength is enhanced by introducing silane coupling agents. The bond strength is enhanced by introducing silane coupling agents. The bond strength is enhanced by introducing silane coupling agents.
### Surface Modification Solutions

**Coupling the Particle to the Application**

**Surface Properties**

<table>
<thead>
<tr>
<th>OLEOPHILICITY</th>
<th>OLEOPHOBICITY</th>
<th>ZETA POTENTIAL</th>
<th>HYDROPHILICITY</th>
<th>HYDROPHOBICITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>OLEOPHILICITY</td>
<td>OLEOPHOBICITY</td>
<td>ZETA POTENTIAL</td>
<td>HYDROPHILICITY</td>
<td>HYDROPHOBICITY</td>
</tr>
<tr>
<td>OLEOPHILICITY</td>
<td>OLEOPHOBICITY</td>
<td>ZETA POTENTIAL</td>
<td>HYDROPHILICITY</td>
<td>HYDROPHOBICITY</td>
</tr>
</tbody>
</table>

**Bonding Mechanisms**

- IONIC BONDING
- METALLIC BONDING
- COVALENT BONDING
- AROMATIC BONDING
- HYDROGEN BONDING
- ACID BASE INTERACTIONS
- INTERCALATION MODIFICATION

**Wetting & Surface Area Effects**

- INTERPENETRATING POLYMERIC NETWORKS

### Chemical Considerations

<table>
<thead>
<tr>
<th>Inputs</th>
<th>Physical Properties</th>
<th>Particle Size &amp; Volume</th>
<th>Particle Size Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>SILICIOUS</td>
<td>Natural</td>
<td>Metallic</td>
<td>Fluorescent</td>
</tr>
</tbody>
</table>

### Solutions

**Adhesive/metal Liquid phase deposition**
- Siloxanes, vinylsilanes, methoxysilanes, and cyclic amine silanes are preferred for small particles and anodized metals. Silane, siloxane, or hydroxy siloxane solutions are prepared containing 5% solids. The systems are then introduced for 3-4 hours until the substrate is treated. It is washed with the solvent. The solvent is then removed by air or explosion oven drying. No further treatment is necessary. The reaction involves a direct metal displacement of the chloride on orifices for metals as evidenced by the surface films. If monolayer or multilayer formation is desired, substrates should be pretreated at 150°C for 4 hours. Each treatment results in absorbed water to prevent oxidation. The method is advantageous for large scale preparations and rigorous controls must be established to ensure reproducible results. More reproducible inorganic or silicas.

**Bulk deposition onto powders**
- Easier treatment is usually accompanied by a spray-on method. The most important step in this process is to ensure that sufficient treated surface is present in the powder that it can be pulverized. The powder is placed in a high intensity fluidized bed, usually with air as the fluidizing medium. The methods are most effective. The final film thickness depends on the time of deposition of the top layer treated material. Such conditions by chemical vapor deposition methods. These methods favor monolayer deposition.

**Vapor Phase Deposition**
- Silane can be applied to substrates using physical vapor deposition techniques. The method can be used for small particles and nanomaterials. The substrates are usually characterized by high quality orifices. The substrates are usually characterized by high quality orifices. The substrates are usually characterized by high quality orifices.

**Surface Modification**
- The substrates are usually characterized by high quality orifices. The substrates are usually characterized by high quality orifices. The substrates are usually characterized by high quality orifices.

**Bonding**
- Silanes are used for inorganic or silicas.

**Hazard**
- Toluene, trichloroethylene, and methanol are used for drying active orifices.
Understanding characteristics that may affect the performance of surface modified micro-particles can dramatically improve the performance in many applications and markets:

**Micro-Particle Surface Modification**

- morphology
- crystal lattice
- polymorphism
- semiconductive
- surface characteristics

**Micro-Particle Dramatic Effects**

- rheological behavior
- hiding power, color strength
- dispersion, solubility, polarity
- photo, chemical, thermal stability
- mechanical & electrical properties
- moisture & corrosion resistance

**For additional information on Gelest’s Surface Modification Technology or to inquire on how we may assist in Enabling Your Technology, please contact:**

11 East Steel Rd.  
Morrisville, PA 19067  
Phone: 215-547-1015  
Fax: 215-547-2494  
micro-particle@gelest.com

www.gelest.com
Surface Modification Solutions for a plethora of applications

- Glass
- Energy
- Textiles
- Displays
- Ceramics
- Digital Inks
- Thermosets
- Biomaterials
- Printing Inks
- Quantum Dots
- Semiconductor
- Thermoplastic
- Chromatography
- Nano-Composites
- Imaging & Printing
- Advanced Composites
- Optics & Optoelectronics

Understanding characteristics that may affect the performance of surface modified micro-particles can dramatically improve the performance in many applications and markets:

**Micro-Particle Properties**
- morphology
- crystal lattice
- polymorphism
- semiconductive
- surface characteristics

**Micro-Particle Dramatic Effects**
- rheological behavior
- hiding power, color strength
- dispersion, solubility, polarity
- photo, chemical, thermal stability
- mechanical & electrical properties
- moisture & corrosion resistance

Gelest, Inc. provides focused technical solutions for surface modification applications and maintains the capabilities to handle flammable, corrosive and air sensitive materials. Headquartered in Morrisville, PA Gelest is recognized worldwide as an innovator, manufacturer and supplier of commercial and research quantities of silanes, metal-organics and silicones, serving advanced technology markets through a material science driven approach.

For additional information on Gelest’s Surface Modification Technology or to inquire on how we may assist in Enabling Your Technology, please contact:

Gelest, Inc.
11 East Steel Rd.
Morrisville, PA 19067
Phone: 215-547-1015
Fax: 215-547-2484
micro-particle@gelest.com

www.gelest.com

© 2009 Gelest, Inc.

Innovating Particle Functionalization